

7 Summary and outlook

At first there is given a short introduction about the influence of chemistry in the agriculture and the possibilities, to fertilise for a long time. New and old products are synthesised and presented in this work, which may have the property of „long time fertiliser“ ,because they have a small solubility.

The behaviour of the solubility has a special interest. While in the gaseous phase the interaction between the molecules can be neglected, the interaction in crystal structure is strong enough, that no change between the molecules is possible. The structure can be determined by X-ray diffraction analysis. In the liquid phase there are many interactions. Therefore the calculation of solubility is very heavy. In this work a qualitative estimation of the solubility is tried to obtain from the crystal structure. Calculation by increments did not lead to result.

There was demonstrated, that urea derivatives can form „polymer structures“ over hydrogen bridges in the solid state analogously to the carboxylic acids. The structures are so strong, that the products are very slightly soluble in water at room temperature. „Polymer structures“ over hydrogen bridges influence the solid-state spectrum because the shielding of atoms by electrons are different and there are no interactions with solvents. That can be an information for the structure.

By ^1H -NMR-spectroscopy could be observed, that at first intermolecular hydrogen bridges are broken, while the intramolecular hydrogen bridges survive for the present. This can be confirmed by calculation with „Spartan“.

For examining the influence of the hydrophobic effect, the solubility of alkylureas was determined. Following this effect, the alkylidiureas can form polyphase systems. Are more than 3 methylene groups at the α,ω -alkylenediureas, the solubility decreases rapid. The reason is, why the hydrophilic of water takes it impossible to invade into the crystal structure. Somewhere has to be examined, if this effect can be transferred at guanidine derivatives as „long-time fertilisers“ with up to 49 % nitrogen.

In the experimental part are synthesized four groups of carbonylureas (the homologous series from urea to the unknown hexauret, ethoxy- and methoxycarbonylurea to the corresponding tetrauret derivatives and acetylurea to acetylbiuret). For the synthesise of methoxy- and ethoxycarbonylurea it was necessary to develop a safe for the preparation of carbonyldiisocyanate. Under special conditions formed trichloronitrogen is destroyed automatically.

Besides of the syntheses of four 3-substituted triuret derivates, other unknown carbonylureas like malon- and succindiureid were synthesized. To get pure products (e. g. prevention of ringformations during the production of malodiureid), it was necessary to work with protection groups. For this reason the amides are reacted with chlorosulfonylisocyanate. The protection group activated the isocyanate group. The chlorosulfonyl group can be hydrolysed in a two step reaction. At first there is produced the sulfamate by HCl-decomposition. The second step is the decomposition of the N-sulfonates under formation of the ureid and sulfuric acid. The intermediate products can be isolated as potassium salts. Their solubilities are similar to these of the amides.

There was to find out, that ethoxy-, methoxycarbonylisocyanate, dichlorophosphorylisocyanate and sulphonyldiisocyanat react in high yields with amide and urea derivatives to carbonylureas.

At all there wehre produced 29 new substances and 19 known substances at new better pathways.